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Review of Heat Transfer Models in GOTH_SNF for Spent Fuel MCO Calculations

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Office of Nuclear Material and Spent Fuel

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Review of Heat Transfer Models in GOTH_SNF for Spent Fuel MCO Calculations

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SUMMARY

The present report is one of a series of three. The series provides an independent technical review of certain aspects of the GOTH-SNF code that is used for accident analysis of the multicanister overpack that is proposed for permanent storage of spent nuclear fuel in the planned repository at Yucca Mountain, Nevada. The work documented in the present report and its two companions was done under the auspices of the National Spent Nuclear Fuel Program. The other two reports in the series are DOE/SNF/REP-087[1] and DOE/SNF/REP-089.[2]

FOREWORD

This report was prepared as the product of a technical review of chemical reactivity modeling and analysis activities performed by the National Spent Nuclear Fuel Program (NSNFP). The scope of the review is contained within the document, "Task Management Agreement for Chemical Reactivity Modeling Technical Review Activities," DOE/SNF/TMA-003. Technical support and administrative leadership for this review work was provided by staff from the NSNFP. The evaluation was conducted by the author of this report, K. W. Childs, who is a staff member of the Computational Sciences and Engineering Division at the Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee.

The NSNFP chemical reactivity analysis provides information about the performance of the multicanister overpack loaded with N-reactor spent fuel in the repository environment relative to the potential for intense chemical reactions on the corroded portions of the fuel elements. The review task was an independent review of the approach and reasonableness of results from the NSNFP chemical reactivity analysis. The chemical reactivity analysis performed by the NSNFP is not a part of the primary licensing strategy for the U.S. Department of Energy spent nuclear fuel in the repository. An additional technical review is not required to meet NSNFP Quality Program requirements. The review discussed in this report was performed as a good technical practice to provide an independent evaluation of the technical adequacy of the NSNFP chemical reactivity analysis. To ensure the technical independence of the review, ORNL personnel conducted the assessment and review to technical standards defined by ORNL without intervention from the NSNFP. NSNFP involvement in the definition of standards and requirements was limited by the requirements outlined in DOE/SNF/TMA-003 to ensuring that work by ORNL personnel was performed under NSNFP procedures, using ORNL personnel as augmented staff. Preliminary review and discussion of results of the evaluation were conducted during the evaluation. This report presents the results of the investigation. NSNFP formal response to recommendations in this report will be documented in a engineering design file, EDF-NSNF-031 "NSNFP Plan for Response Activities to Chemical Reactivity Review Recommendations".

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1. INTRODUCTION

This report examines the heat transfer mechanisms occurring within the multicanister overpack (MCO) and reviews assumptions and simplifications made in developing the GOTH_SNF MCO model. The comments are based primarily on information obtained from two INEEL reports.[3,4] but are influenced by additional information obtained during conference calls with R. L. Bratton.[a,b]

2. HEAT TRANSFER MECHANISMS

This section examines the three mechanisms for transferring heat within the MCO: radiation, conduction, and convection. The following are some points of specific interest from the conference calls. (1) During an accident transient the primary path for heat removal from the interior is radial transport to the MCO wall via thermal radiation, gas conduction, and natural convection loops within individual baskets. Heat is then rejected from the MCO outer surface to the surroundings. Furthermore, transport by thermal radiation is by far the dominant mechanism. (2) Convective cooling due to airflow through the MCO is not a significant heat removal mechanism. These points are important to the understanding of the behavior of the MCO during an accident, and they should be discussed in the documentation.

2.1 Radiation

The GOTH_SNF analyses indicate that the dominant mechanism for transporting heat from the interior of the MCO to the MCO outer wall is thermal radiation. Therefore, it is important to have an accurate representation of radiation heat transfer in the modeling. The geometric approximation for the fuel elements used in GOTH is shown on the left side of Figure 1. In the GOTH approximation, radiation heat transfer occurs between the outer surface of a fuel ring and the inner surface of the next fuel ring. On the right side of the figure, the true geometry is shown. The fuel elements that are consolidated into fuel ring 1 are identified as are those for fuel ring 2. Also highlighted are the surface areas associated with the outer surface of fuel ring 1 and the inner surface of fuel ring 2.

Heat transfer between two surfaces that exchange heat by thermal radiation with each other and nothing else is given by:

$$q_{net} = \frac{\sigma(T_1^4 - T_2^4)}{(1-\varepsilon_1)/\varepsilon_1 A_1 + 1/A_1 F_{12} + (1-\varepsilon_2)/\varepsilon_2 A_2}.$$

Consequently, for given values of surface temperature, the net heat transfer between the surfaces is proportional to a factor given by:

$$f_r = \frac{1}{(1-\varepsilon_1)/\varepsilon_1 A_1 + 1/A_1 F_{12} + (1-\varepsilon_2)/\varepsilon_2 A_2},$$

a. Conference call with R. L. Bratton et al., Idaho National Engineering and Environmental Laboratory, June 23, 2003.

b. Conference call with R. L. Bratton et al., Idaho National Engineering and Environmental Laboratory, August 6, 2003.

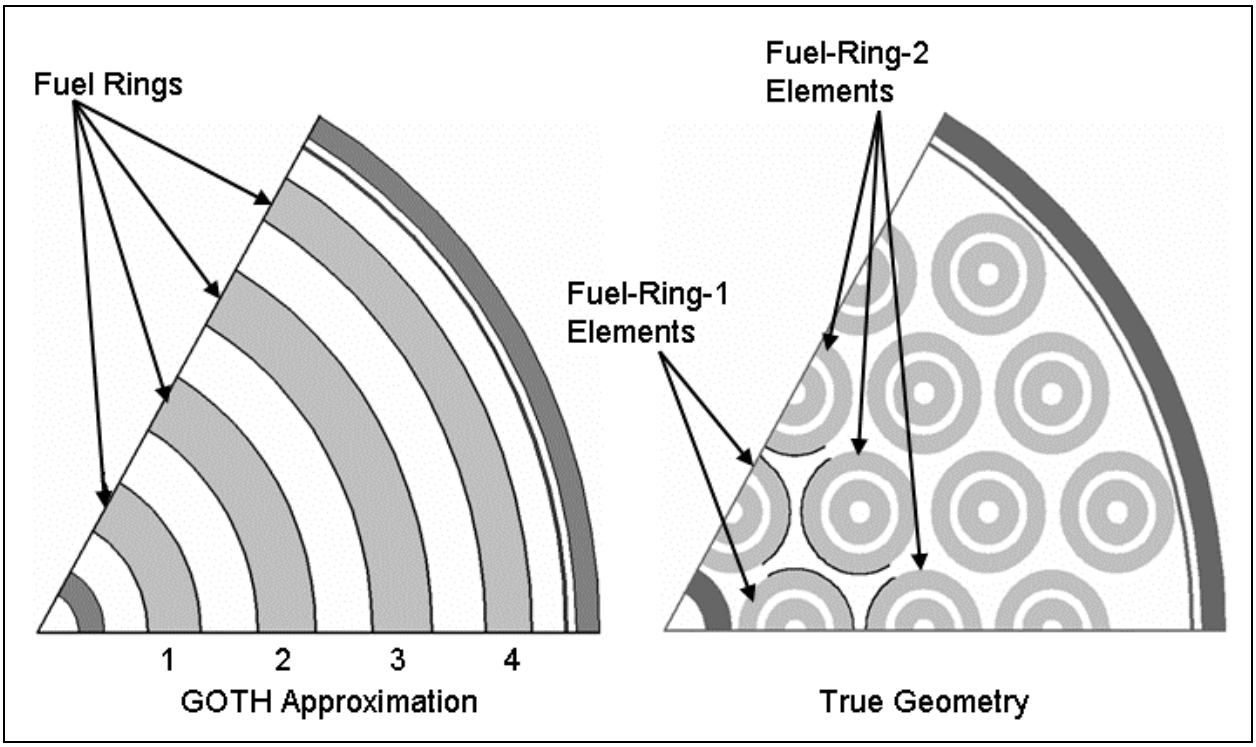

Figure 1. Axisymmetric approximation and true geometry for radiant exchange within MCO.

where

ε_i = emissivity of surface

A_i = area of surface

F_{12} = view factor (exchange factor) from surface 1 to surface 2.

For the fuel ring approximation, the view factor from the outer surface of a ring to the inner surface of the next outer ring is 1.0. Using an emissivity of 0.3 for both surfaces, the outer surface area of fuel ring 1 and the inner surface area of fuel ring 2, the factor f_r is calculated to be 0.3604. In order to see how this compares to f_r for the actual geometry, the simplifying assumption is made that the small gaps between fuel elements have a negligible impact on the radiation heat transfer (i.e., the surfaces highlighted in image on the right side of Figure 1 can see only each other and no other surfaces.) The view factor from the fuel element surfaces associated with the outer surface of fuel ring 1 to the fuel element surfaces associated with the inner surface of fuel ring 2 is approximately 0.67. (This view factor was determined using Hottel's crossed-string method. However, it is still an approximation because it was done by literally measuring the length of strings laid on an image of the fuel elements rather than performing rigorous geometric calculations.) Using the stated approximations, the factor f_r for the actual configuration is calculated to be 0.4461. The factor f_r is greater for the actual configuration than it is for the approximation using fuel rings. This means that the axisymmetric GOTH model is conservative (i.e., the model will overpredict temperatures in the interior of the cask).

The above discussion assumes that the GOTH model uses the fuel ring surface areas rather than the true fuel element surface areas although the method used for surface area calculations is not explicitly stated. The fuel ring surface areas are less than the true surface areas of the fuel elements. For the flow/convection model, there is a correction factor applied to the ring surface area to bring it into agreement with the true surface area. If a similar correction is applied to the ring surface areas for the radiation calculation, then the factor f_r is 0.4884 for the GOTH model. If true fuel element surface areas and a view factor of 1.0 are used in the GOTH model, then the model is not conservative. It overpredicts heat transfer from one fuel ring to the next by approximately 9.5%.

The Zircaloy-2 cladding on the fuel elements is neglected in the model. This is a reasonable assumption when considering thermal conduction because the layer is thin and represents a negligible resistance to heat transfer and also a negligible heat capacity. However, for heat transfer due to thermal radiation, the emissivity of the fuel element surface is a key factor. This is very important because thermal radiation is the primary mechanism for transporting heat from the interior to the outer shell of the MCO. To be conservative, the model should use the lowest credible emissivity for the surfaces of the fuel elements. In Reference 3, Section 7, MCO Material Property Data, an emissivity for oxidized uranium is listed, but emissivities are not listed for Zircaloy-2 or unoxidized uranium. One would infer from this that the modeler assumes that the Zircaloy-2 cladding is ruptured by corrosion so that the entire exposed surface of the fuel elements is oxidized uranium metal. If so, the documentation should be altered to make that point explicitly. If it is credible to have either Zircaloy cladding or exposed unoxidized uranium metal, then the one with the lowest emissivity should be assumed. The documentation needs to clearly state and justify the emissivity that is used for the surfaces of the fuel elements

If heat removal due to airflow through the MCO is indeed negligible, then any heat generation associated with the inner portion of a fuel element must be transported across the annular space between the inner and outer portions of the fuel element by gas conduction and thermal radiation. The model neglects the resistance to heat transfer due to the gap between the inner and outer fuel elements. Neglecting this gap resistance may lead to an underestimation of the maximum temperature occurring in the uranium. Because the gaps cannot be included in the axisymmetric model, auxiliary calculations should be performed to obtain an upper-limit estimate of the temperature difference across these gaps to see if neglecting them is justified. This issue is discussed further in the section on conduction heat transfer.

2.2 Conduction

GOTH_SNF calculations indicate that the second most important heat transfer mechanism for removing heat from the interior of the MCO is radial conduction through a path consisting of a combination of metal of the fuel elements and intermediary air. In GOTH_SNF, all the metal in the fuel elements is lumped into rings whose volumes are the sums of the elements lumped into the particular ring. Figure 2 shows a single fuel element on the left and the portion of a fuel ring corresponding to a single element on the right. The air volume between fuel elements is also modeled as annular rings. The annular ring approximation does not accurately model the conduction path in either the metal or the air, and it is not immediately obvious how this approximation affects heat conduction.

Radial heat conduction is calculated using the resulting radial thicknesses and the conductivity of uranium metal whereas the true conduction path through the elements is more complex than this. Among other things, the inner elements, which contain roughly one-third of the uranium, are partially isolated from the outer elements by the air gap between the inner and outer elements. The conduction paths should be examined in more detail, and a basis for radial conductance across a ring should be developed. One approach for doing this is outlined below.

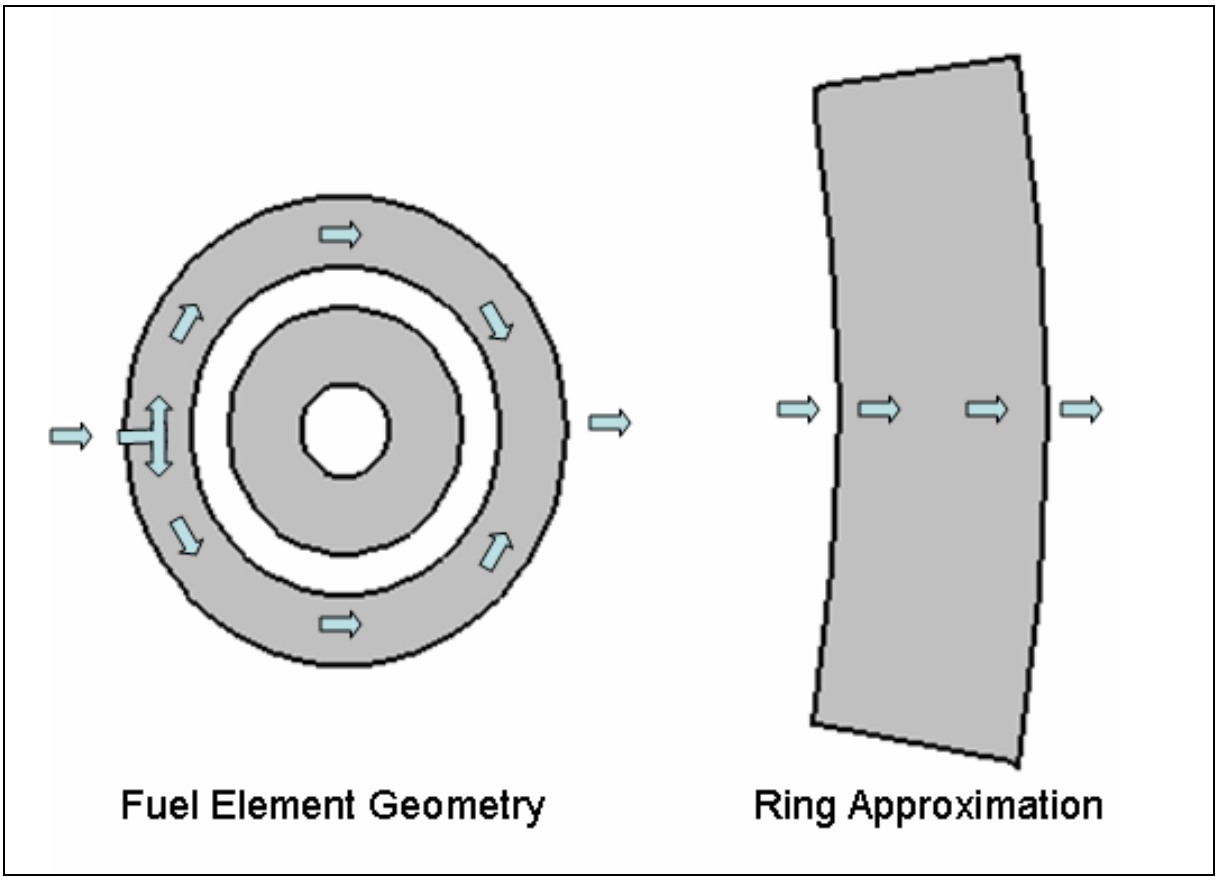

Figure 2. True fuel element geometry and ring approximation.

To demonstrate one method for developing an effective conductivity for the uranium in a fuel ring, conduction from fuel ring 1 to fuel ring 2 is examined. The image on the left side of Figure 3 shows a one-sixth symmetry section of a fuel basket. For the purpose of this discussion, it is assumed that heat is being conducted from the center to the outer surface of the MCO, but no heat generation is occurring in the fuel elements themselves. Under these conditions it seems reasonable to assume that the line passing through the center of the elements that compose fuel ring 1 is approximately isothermal; and, likewise, the line passing through the elements composing fuel ring 2 is also isothermal. The image on the right side of Figure 3 shows the smallest repeating pattern in the area between the isothermal lines. Because of symmetry, two of the surfaces can be assumed to be adiabatic. A finite-element or finite-difference heat transfer code (subsequently referred to as the numerical model) can be used to determine the heat flow per unit length of fuel element for an assumed temperature difference across this model. The heat flow from this model must be multiplied by twelve to get the total heat flow from elements in fuel ring 1 to the elements in fuel ring 2.

Heat transfer from the center of the first fuel ring to the center of the second fuel ring can be calculated from the equation

$$q = \frac{2\pi(T_1 - T_2)}{ln(r_{1out}/r_{1cen})/k_{Ueff} + ln(r_{2in}/r_{1out})/k_{air} + ln(r_{2cen}/r_{2in})/k_{Ueff}}$$

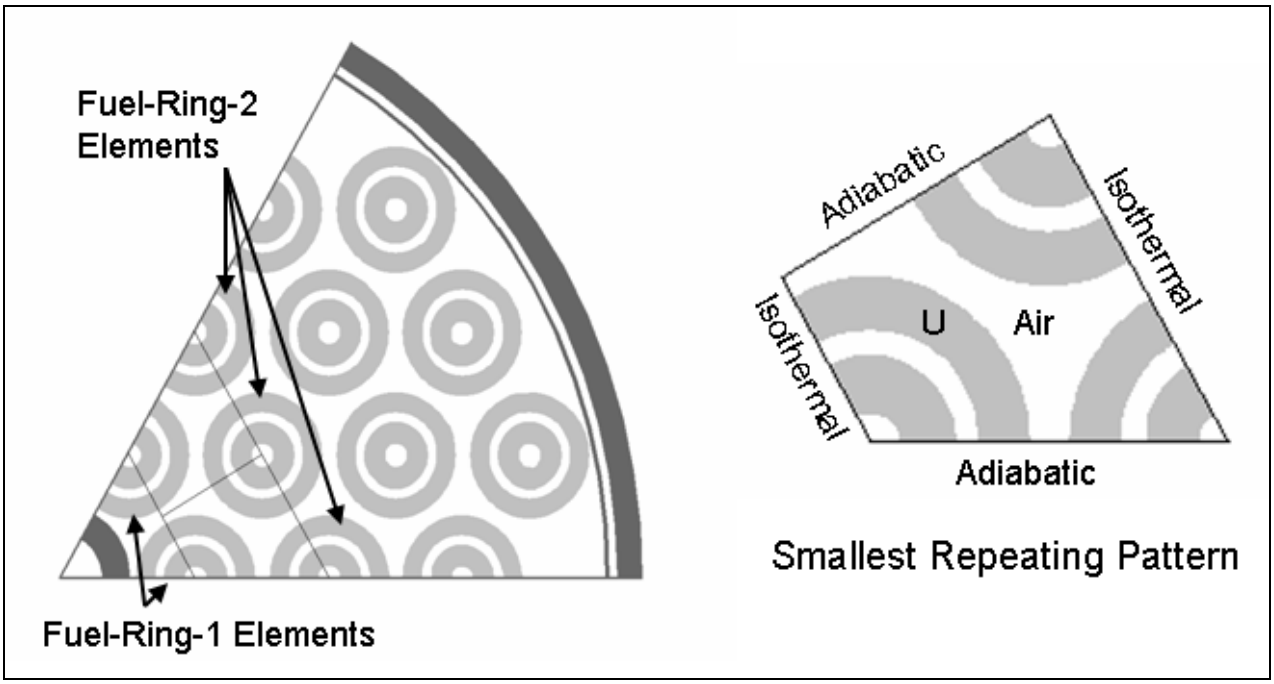

Figure 3. Detailed model for radial heat conduction.

where

q = heat flow per unit length of fuel element (Btu/h-ft)

$T_1 - T_2$ = temperature difference used in previous numerical model (°F)

r_{1out} = outer radius of 1st fuel ring (ft)

r_{1cen} = radius at the center of 1st fuel ring (ft)

r_{2in} = inner radius of 2nd fuel ring (ft)

r_{2cen} = radius at the center of 2nd fuel ring (ft)

k_{air} = thermal conductivity of air (Btu/h-ft-°F)

k_{Ueff} = effective thermal conductivity of uranium (Btu/h-ft-°F).

Using the heat flow and temperature difference from the numerical model, the above equation can be solved for the effective conductivity of uranium. A similar procedure should be repeated for heat flow from the second to the third fuel ring and for heat flow from the third to the fourth fuel ring to determine the effective uranium conductivity for each. If the smallest effective uranium conductivity determined from this procedure is greater than or equal to the actual conductivity of uranium, then the axisymmetric GOTH_SNF model is a reasonable, or perhaps even conservative, approximation of radial conduction in the MCO. However, if the smallest effective uranium conductivity determined from this procedure is less

than the actual conductivity of uranium, then the axisymmetric GOTH_SNF model is not a conservative approximation of radial conduction in the MCO. In this case, some of the GOTH_SNF MCO calculations should be repeated using the lowest effective uranium conductivity (or alternatively, a different effective conductivity for each ring) to determine how much impact this has on the results. Using a smaller effective thermal conductivity will also impact axial conduction, but it is more important to accurately model heat transfer in the radial direction because this is the primary heat flow direction.

Using an effective uranium thermal conductivity should be a reasonable model for gross radial heat flow from element to element, but it may not capture the maximum temperature in the inner portion of the fuel element. Because of resistance to heat flow across the gap, the inner portion of the fuel is somewhat thermally isolated from the outer portion of the fuel element. An upper limit on the inner element fuel temperature can be obtained fairly easily. Taking the maximum heat generation rate in the inner portion (heat of reaction plus decay heat) and the maximum temperature at that time in a fuel ring, the temperature of the inner fuel element surface necessary to transport the heat across the gap via combined conduction and radiation can be calculated.

2.3 Convection

There are three distinct natural convection loops that have the potential for forming within the MCO. First, for a two-hole breach of the MCO, air can enter the lower hole, flow up through the fuel baskets, and exit out the upper hole. Second, an internal loop can form within the confines of a single fuel basket; and, third, an internal loop can form that spans more than one fuel basket. Each of these will be discussed individually in the following paragraphs.

On casual examination, one might expect that the convective flow through the MCO following a two-hole breach is a significant mechanism for heat removal; however, the GOTH_SNF results indicate this is an insignificant heat removal mechanism. Nonetheless, the accuracy of the model should still be investigated. The consolidation of multiple fuel elements into contiguous fuel rings in the axisymmetric model alters the flow path through the fuel baskets. There are three flow paths associated with each fuel element where it sits in the socketed aluminum plate: the center hole in the inner portion of fuel element, the annular space between the inner and outer portions of the fuel element, and the annular space between fuel element and the aluminum plate. This is handled in the GOTH_SNF MCO model with a loss coefficient for the socketed aluminum plate based on the combined flow area for these three paths. This model would be accurate only if all the paths recombined just above the socketed aluminum plate, which they do not. The flow paths internal to a fuel element do not rejoin the flow on the outside of the fuel elements until they reach the space above the top of the fuel elements.

To determine the flow distribution amongst the three flow paths associated with a fuel element, a finite element model was developed at ORNL using the commercial CFD code, CFdesign. The vertical air flow enters at the bottom of each basket through a number of holes in the base plate. The position of the holes in the base plate relative to the position of individual fuel elements is shown in Figure 4. It can be seen in this figure that there are two holes in the base plate associated with each fuel element. The volume included in the finite element model extends vertically from the centerline of the base plate of one fuel basket to the centerline of the base plate of the next fuel basket above and is shown in Figure 5. The model includes the air volume within and surrounding a fuel element, but does not include the solid portions of the fuel element or basket. Flow enters through the two holes in the base plate at the bottom of the model and exits through the two holes in the base plate at the top. The outer surface of the flow path associated with flow outside the fuel element is approximated as a circle with the area matching the actual hexagonal area associated with this flow. The model has a free-slip boundary condition applied on this outer surface (i.e., the model does not allow cross flow between fuel elements). The model was run for one pressure difference and the flow in each of the three channels was examined at mid-height of the

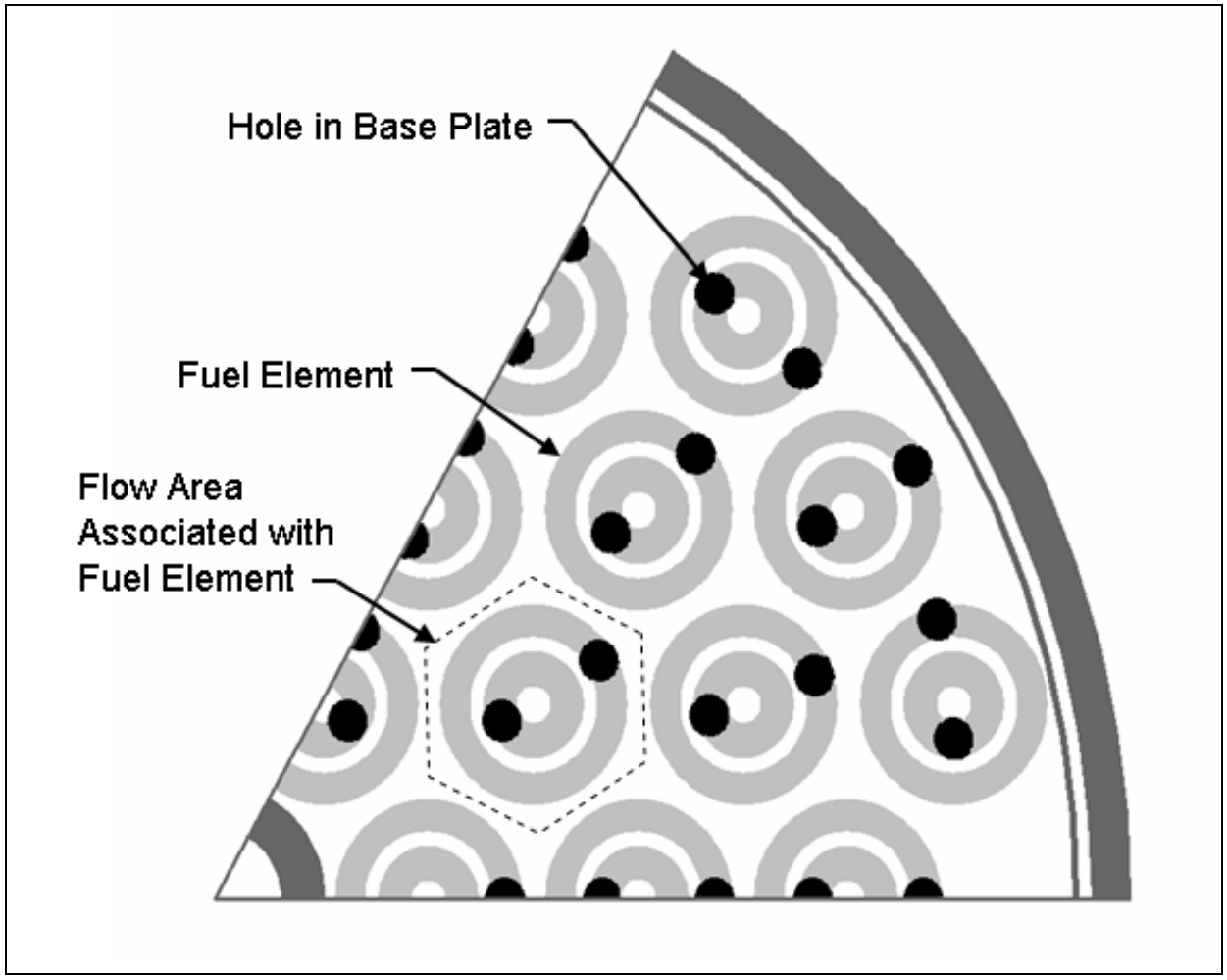

Figure 4. Position of base-plate holes relative to fuel elements.

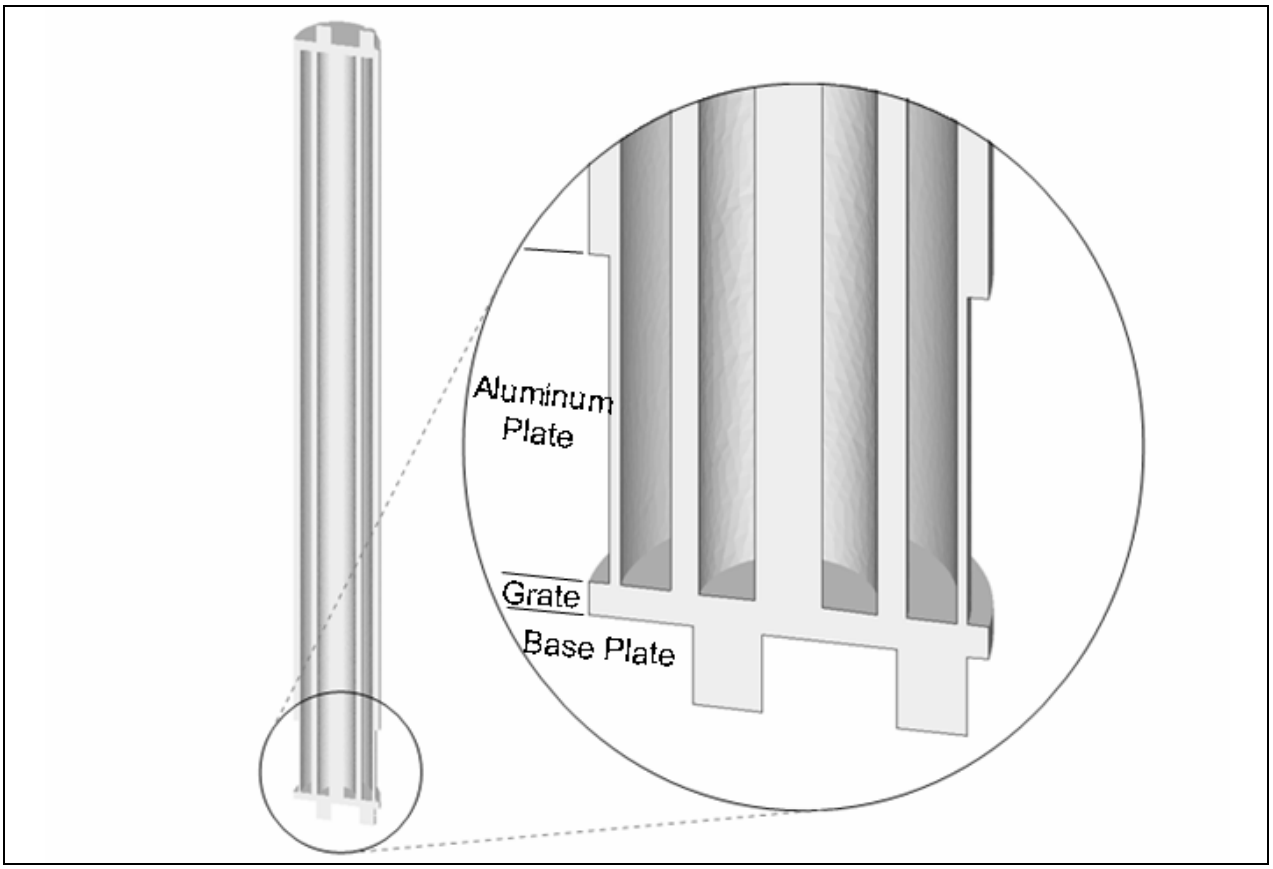

Figure 5. Flow model for vertical flow through/around fuel elements.

model. The results show that just over half of the flow is in the channels within the fuel element. The breakdown is 12.9% for the center hole, 37.6% for the annular gap, and 49.5% for the area outside the fuel element. When compared to the velocity in the area outside the fuel element, the velocity in the annular gap is 45% higher, and the velocity in the inner hole is three times as large. The axisymmetric MCO model represents these three distinctly different flow paths with a single flow velocity. The low relative velocity and mass flow on the outside of the fuel elements is because of the flow resistance of the small gap between a fuel element and the socketed aluminum plate.

The two-dimensional GOTH_SNF model does not include heat removal from the surfaces of the internal flow passages in the fuel elements. The surface area for heat removal in the model matches the outside surface area of the fuel elements. Neglecting heat transfer from these surfaces might result in the model overpredicting the maximum temperature in the uranium; but temperatures, convective flow rates, and reaction rates are so interconnected that this cannot be stated with any degree of certainty.

Because results from transient accident calculations show that airflow through the cask is not a significant heat transfer mechanism, accurate modeling of this heat removal mechanism may not be essential from that standpoint. However, an accurate flow model is important for an accurate chemical reactivity model because this flow supplies oxygen to the reaction and transports reaction products. Holes in the base plates are positioned to provide airflow to the inner flow passages within fuel elements as well as flow to the space between fuel elements. The purpose of these holes is presumably to enhance heat transfer via natural convection flow. But, in light of the results from the analyses, they may actually serve primarily to supply oxygen to the reactions occurring following an MCO breach. There is a possibility

that the presence of the base plate flow holes may actually increase reaction rates and, consequently, make maximum temperatures higher during an accident.

A three-dimensional GOTH_SNF model of the MCO is in development. When completed, this model can be used to benchmark the current two-dimensional model to determine if a more accurate model of these flow paths significantly impacts the results.

Within each fuel basket, a convective loop can form in the volume outside the fuel elements that are bounded by the socketed aluminum plate on the bottom and the base plate for the next higher fuel basket on the top. The flow in the internal channels in the fuel elements does not participate in this natural convection loop. The GOTH_SNF MCO two-hole-breach calculations indicate that the velocities occurring in this convective loop are significantly higher than those of the flow through the MCO. Because the through flow is small, the combining of the flow in the internal fuel element passages with that outside the element should not have a significant impact on this convective loop. The model used is a reasonable approximation of this mechanism.

The internal flow passages within fuel elements can only participate in a natural convection loop if the loop spans the base plate for the fuel basket. This does not appear to be a significant mechanism for heat transfer in the MCO.

3. CONCLUSIONS AND RECOMMENDATIONS

The primary recommendation is that the documentation needs to be expanded to clearly state assumptions that have been made and present a justification for them. Specifically:

1. Assumptions made in the modeling of thermal radiation need to be clearly stated and justified. Assumptions needing clarification are the emissivity for the surface of the fuel elements and the radiation surface areas used.

2. Additional calculations need to be performed to determine an effective thermal conductivity for the fuel rings to ensure that the model is accurate. A suggested procedure for doing this is presented in this report.

3. A verification that the axisymmetric flow ring model accurately predicts flow within the MCO is needed. This can be accomplished by using the three-dimensional model that is in development to benchmark the two-dimensional calculations.

A general discussion of the results of the calculations needs to be included in the report. The conclusions that thermal radiation is the primary mechanism for heat removal and that convective flow through the MCO is an insignificant mechanism for heat removal are surprising results. These points are important to the understanding of the behavior of the MCO during an accident and should be discussed in the documentation.

3.1 NSNFP Evaluation and Response to Review Recommendations

The author of this report consulted with the NSNFP during his evaluation of the computer modeling. Several items were resolved and clarified during these consultations. Preliminary review and discussion of results of the evaluation were also conducted during these consultations. This report contains recommendations for future action by the NSNFP. The NSNFP formal response to the recommendation in this report will be documented in a future engineering design file, EDF-NSNF-031, “NSNFP Plan for Response Activities to Chemical Reactivity Technical Review Recommendations.”

4. REFERENCES

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